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IUCr Newsletter

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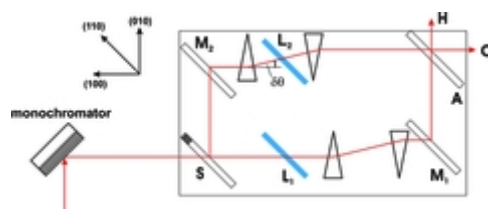
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A neutron interferometric measurement of a phase shift induced by Laue transmission

***Acta Cryst.* (2010). A66, 17–21 (doi.org/10.1107/S010876730904522X)**



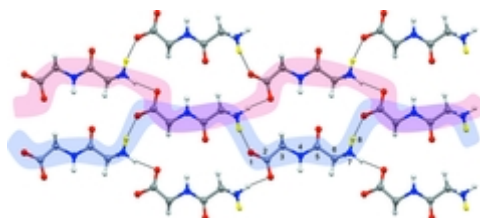
Interferometer set-up for measurement of a phase shift by dynamical neutron diffraction

A neutron beam incident on a perfect crystal close to a Bragg condition is not only split into a transmitted and a reflected beam but also shows a distinct phase shift in the transmitted direction. The most pronounced feature is an extreme angular phase sensitivity of the order 1° phase shift per 10^{-4} arcsec beam deviation. Another interesting aspect is the occurrence of Pendellösung structures in the phase progress. A measurement of this phase shift has been performed by an especially developed neutron interferometer.

J. Springer, M. Zawisky, H. Lemmel and M. Suda

Structures of dipeptides: the head-to-tail story

***Acta Cryst.* (2010). B66, 84-93 (doi.org/10.1107/S0108768109053257)**



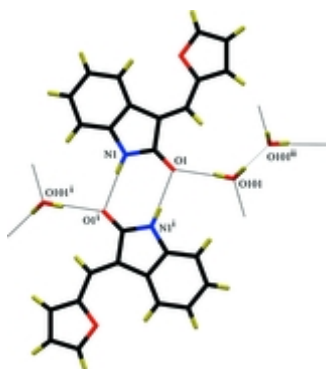
The simultaneous presence of two crystallographically independent hydrogen-bonded chains, highlighted in blue (with yellow H atoms) and red, in a dipeptide structure. Peptide side chains have been omitted. Hydrogen bonding in crystal structures of unprotected, zwitterionic dipeptides is dominated by head-to-tail chains involving the amino and carboxylate groups. Of special interest are patterns with two concomitant chains that generate a hydrogen-bonded layer. A comprehensive survey shows that these can conveniently be divided into only four groups, differing not only in the symmetry of the chains and amide hydrogen bonding, but also in peptide conformation and the propensity to include guest molecules. The pattern observed for a specific dipeptide follows from the amino-acid sequence.

C. H. Görbitz

IUCR JOURNALS NEWS

Seven 3-methylidene-1*H*-indol-2(3*H*)-ones related to the multiple-receptor tyrosine kinase inhibitor sunitinib

***Acta Cryst.* (2010). C66, o71-o78 (doi.org/10.1107/S0108270109054134)**



The structural features of the compounds presented in the solid state correlate strongly with those found in solution. For example, stereoisomer characterisation [(*E*)- or (*Z*)-] and the presence of intramolecular hydrogen bonding are confirmed by both techniques although the X-ray study reveals extended intermolecular hydrogen bonding, which is not observed in solution-based techniques (^1H NMR). The predominant motif in the crystal structures is that of intermolecular hydrogen bonding (N–H...O=C) between the 1*H*-indol-2(3*H*)-one units. This motif is maintained in the one structure that contains a hydrogen-bonding hydrate molecule. However, one structure, methyl 3-(1-methylethylidene)-2-oxo-2,3-dihydro-1*H*-indole-1-carboxylate, a carbamate analogue lacking an N–H bond, displays no intermolecular hydrogen bonding.

J. Spencer, B. Z. Chowdhry, S. Hamid, A. P. Mendham, L. Male, S. J. Coles and M. B. Hursthouse

IUCR JOURNALS NEWS

MolProbity: all-atom structure validation for macromolecular crystallography

***MolProbity*: all-atom structure validation for macromolecular crystallography**

***Acta Cryst.* (2010). D66, 12-21 (doi.org/10.1107/S0907444909042073)**



The *MolProbity* web service will diagnose most local errors in protein or nucleic acid crystal structures and help guide their correction. It uses optimized hydrogen placement and all-atom contact analysis to identify physically impossible steric 'clashes', complemented by updated versions of geometric and torsion-angle criteria, presented as sortable charts and interactive 3D graphics. This article reviews *MolProbity* features, reports on recent enhancements, and presents evidence that the resulting improvements are beneficially affecting the global database.

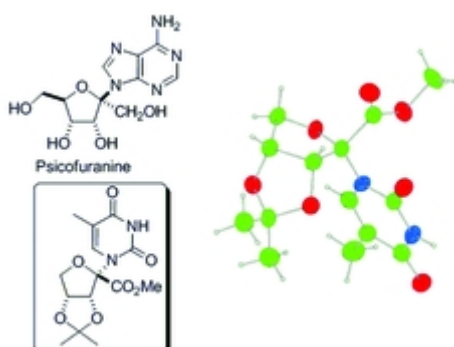
V. B. Chen, W. B. Arendall, J. J. Headd, D. A. Keedy, R. M. Immormino, G. J. Kapral, L. W. Murray, J. S. Richardson and D. C. Richardson

IUCR JOURNALS NEWS

1-(1-Carboxymethyl-1,4-anhydro-2,3-O-isopropylidene- α -d-erythrofuranosyl)thymine

1-(1-Carboxymethyl-1,4-anhydro-2,3-O-isopropylidene- α -d-erythrofuranosyl)thymine

Acta Cryst. (2010). E66, o404 (doi.org/10.1107/S1600536810001704)



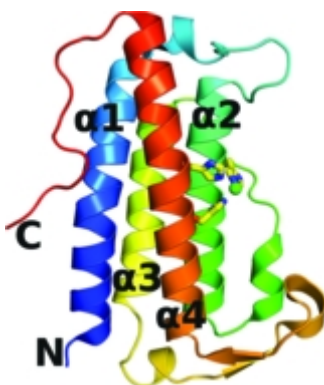
Psicofuranine is a naturally occurring branched-sugar nucleoside which exhibits potent biological activity; however, it is cardiotoxic to man. In studies to synthesise analogues of psicofuranine and evaluate their biological potential, methodology was developed to introduce the nucleoside base *via* a Vorbrüggen-type displacement on a carbohydrate-derived α -bromoester. α/β selectivity is extremely important for biological activity and X-ray crystallography has been invaluable to unequivocally assign the stereochemistry of the nucleoside base.

G. M. J. Lenagh-Snow, S. F. Jenkinson, A. J. Stewart, G. W. J. Fleet and D. J. Watkin

The structure of DinB from *Geobacillus stearothermophilus*: a representative of a unique four-helix-bundle superfamily

The structure of DinB from *Geobacillus stearothermophilus*: a representative of a unique four-helix-bundle superfamily

Acta Cryst. (2010). F66, 219–224 (doi.org/10.1107/S1744309109053913)



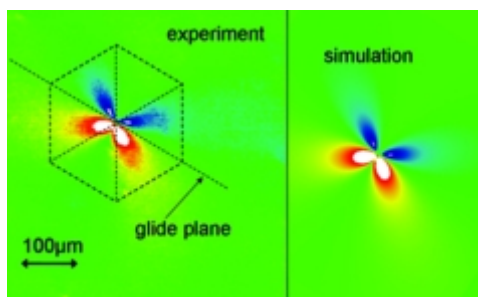
Ribbon diagram of a monomer of DinB colored with a spectrum from the N-terminus (blue) to the C-terminus (red). The Ni^{2+} -coordinating histidine triad is shown as sticks and the Ni^{2+} ion is shown as a green sphere.

Geobacillus stearothermophilus DinB (GsDinB) is a dimer encoded by a DNA damage-induced gene under the control of the SOS-like repair systems. Monomers consist of an unusual up–down–down–up four-helix bundle with the α_1/α_2 loop crossing over the top of the bundle and the α_3/α_4 loop wrapping under the bundle. GsDinB contains a metal-binding histidine triad motif. Structural similarity searches reveal a small yet diverse clan of Pfam families containing this fold. At least four different quaternary structures, including three dimerization architectures, have been observed.

D. R. Cooper, K. Grelewski, C.-Y. Kim, A. Joachimiak and Z. S. Derewenda

Micropipe-induced birefringence in 6H silicon carbide

J. Appl. Cryst. (2010). 43, 122-133 (doi.org/10.1107/S0021889809043957)

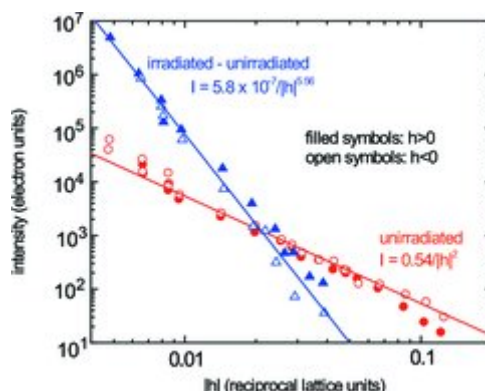


Experimental (left) and simulated (right) birefringence image of a micropipe from a 6H-SiC wafer. The refractive index is a function of materials strain, and observing the birefringence around dislocations may reveal useful information. The dislocation core is in the range of angstroms, but the stress field can extend over tens of micrometers and becomes accessible to optical microscopy. We showed that the birefringence of well known defects such as silicon carbide micropipes can be put on a quantitative footing, and we were able to identify and fully reproduce the birefringent patterns. This technique is cheaper than transmission electron microscopy or X-ray topography.

T. Ouisse, D. Chaussende and L. Auvray

X-ray microdiffraction analysis of radiation-induced defects in single grains of polycrystalline Fe

J. Synchrotron Rad. (2010). **17**, 250–256 (doi.org/10.1107/S0909049509052078)



Excess scattering from irradiated polycrystalline Fe and total scattering from an unirradiated control sample, both cooled to 77 K to reduce thermal scattering.

Diffuse X-ray scattering has long been used to analyze lattice defects. Until now, mm-scale single crystals have been required for high-quality results. By focusing synchrotron X-rays to a micron-scale focus, comparable results are obtained from a single grain in a polycrystalline sample. This novel technique will enable the study of materials which cannot be grown as single crystals. Highly radioactive materials may now be studied more safely by using very small samples.

E. D. Specht, F. J. Walker and W. Liu

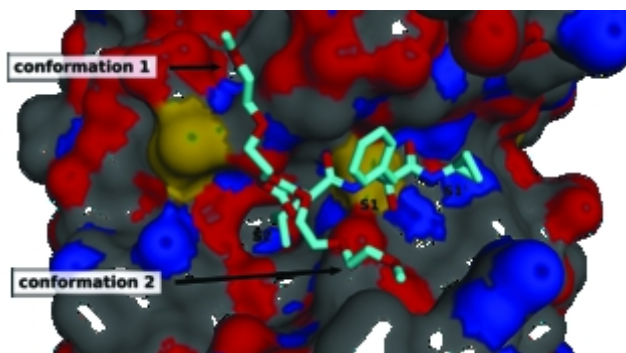
MEETING REPORT

ACA 2009

Toronto, Ontario, Canada, July 2009, www.amercrystalassn.org

Below is a summary of the report that appeared in *ACA Reflexions*, Fall 2009, pp. 10-46.

The 2009 ACA meeting (Local Chair: David Rose (Waterloo) – Program Chair: Jim Britten (McMaster)) had the third largest attendance ever with over 1000 registrants and exhibitors.



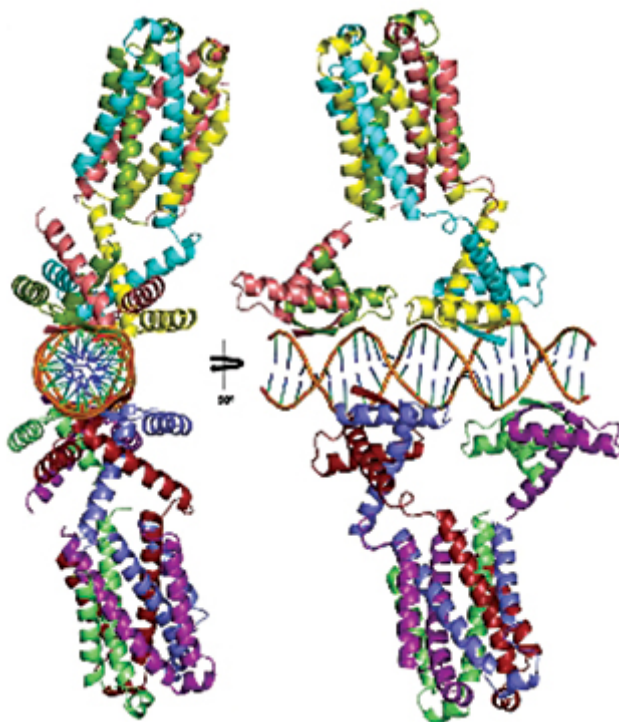
Calpastatin bound to the active site of calpain 2; an inspiration for the design of calpain inhibitors. Kristin Low, ACA09 Pauling Poster Prize winner.

Plenary Lectures: Ted Baker (U. of Auckland) gave a historical lecture that began by citing Louis Pasteur who first demonstrated that external form reflects internal structure. His talk cataloged the work of pioneers in crystallography and connected molecular structure with biology, chemistry, mathematics, art and architecture. Philip Coppens (SUNY, Buffalo) discussed the supramolecular solid state as a medium for photochemical studies of molecules. Shih-Lin Chang (Warren Award – National Tsing Hua U.), discussed coherent dynamical interactions in X-ray multiple diffraction and crystal cavity resonance. Svilen Bobev (Etter Early Career Award – U. of Delaware) presented his work on novel germanide structures. Michael James (Buerger Award – U of Alberta) took his audience on a journey from his early 'exposure' to X-rays at the U. of Manitoba and his doctoral studies with Dorothy Hodgkin at Oxford through his time in Alberta winding up with his present research on proteins in *Mycobacterium tuberculosis*.

Transactions Symposium: Speakers concentrated on phase transitions, a rigorous arena for studying the balance of forces that stabilize particular atomic conformations, with direct applications in pharmacology and drug design where stable polymorphs are critical, and in the design of devices to monitor and control technological properties.

'Would You Publish This?': Presenters 'aired their dirty laundry' in an effort to stimulate discussion about how small molecule crystallographers handle problem crystal structures of chemical importance. Issues of disorder, solvent loss, and inherently bad data were discussed. J. Tanski (Vassar College) described a structural model considered 'bad' by IUCr standards that was still useful to chemists. F. Fronczek (Louisiana State U.) presented 'Barely Publishable' porphyrin structures that were barely solvable and nearly impossible to refine yet provided critical chemical information. Subsequent discussion topics included: (a) the effort required to generate incremental improvements in structure quality, (b) methods to ensure the experimental details are included in the publication by the chemist, and (c) when is the program *Squeeze* appropriate and does it bias the structural model? 'Would You Publish This II?' is scheduled for the ACA 2010 in Chicago.

Small molecule problem structures: Talks addressed the benefits of using the synchrotron sources for twinned and/or highly disordered crystals, C. Beavers (Advanced Light Source, LBNL), and exploiting pseudo-symmetry in crystal structures that have a high Z' value, V. Young (U. Minnesota).



The crystal structure of a TraM-DNA complex from the F-related plasmid pED208. (Joyce Wong, U. Alberta)

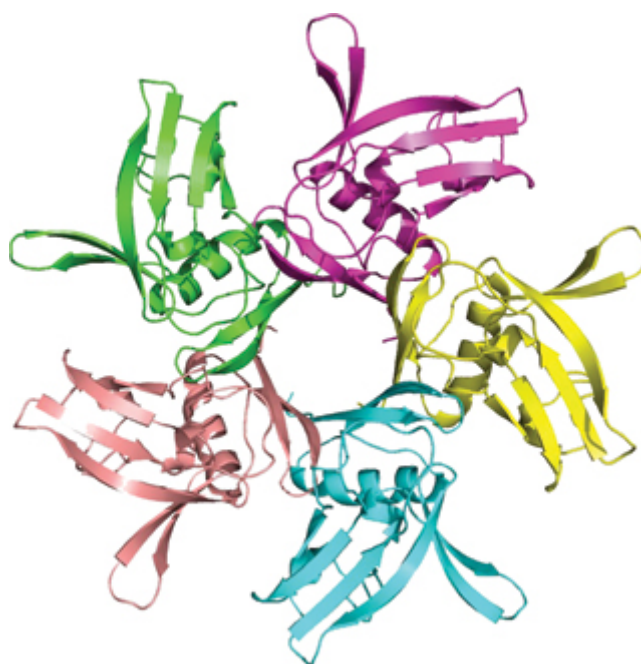
Supramolecular Chemistry: Topics included intermolecular forces, non-covalent assemblies, crystal growth, materials design, pharmaceuticals, and database studies. G. Desiraju (Indian Inst. of Science) offered an insightful look at polymorphism and structures with high Z' , as well as a spirited defense of the relevance of small-molecule crystallography. Other talks included: Halogen bonding, P. Metrangola (Politecnico de Milano); host-guest chemistry, J. Wuest (Montreal); solid-state based photochemistry, M. Kaftory (Technion) and D.-K. Bucar (Iowa), and co-crystals of pharmaceutically active ingredients, S. Forbes (Kansas State) and H. Abourahma (College of New Jersey).

Professional Directions: A panel of six crystallographers (S. Ginell, Argonne Labs; J. Kaduk, INEOS Technologies; S. Sheriff, Bristol Myers-Squibb; C. Stern, Northwestern U.; P. Swepston, Rigaku Americas; C. Wilmot, U. of Minnesota; and M. Wilson, U. of Nebraska-Lincoln) answered the question 'Is there a future for crystallography?' with a resounding 'YES!' In answer to concerns about career options in crystallography in the current tumultuous economy the panel's advice was to pursue a career that you are passionate about. They stressed that a willingness to accept change affords great opportunities. A common theme among the personal stories of the panelists was that each had a supportive mentor. This theme accentuated the importance of seeking out collaborations and building relationships. A similar session, 'Professional Odysseys', aimed at informing young scientists of career options and advancement opportunities will be held in Chicago.

Educational Outreach: Presentations included descriptions of Protein Data Bank (PDB) activities for dissemination of structural data to students, educators and the general public, C. Zardecki and S. Dutta (RCSB PDB); the internet as a forum for communication, discussion and tutorials about crystallography, S. Seaver, (Toledo - www.P212121.com); and a free online teaching set of the Cambridge Structural Database (CSD) for use in undergraduate chemistry curricula, G. Battle (CCDC). Buffalo high school students discussed the possibility of a primordial genetic code. By analyzing codon use in the ancient bacteria *Anaeromyxobacter dehalogenans* they concluded that 3 billion years ago, a precursor to the standard genetic code used 32 codons, all ending in G or C, to encode all amino acids. B. Rupp (Q.E.D.

Life Sciences) advocated the use of real molecules to help students make the connection between crystallography, symmetry, and real life problems. L. Malaspina (U. Federal de Goiás) described her experiences attending the 2009 ACA Summer School, bringing samples, collecting data, and working on data analysis with experts in the field.

Vaccine Design: I. Wilson (Scripps), B. Baker (Notre Dame), and R. Rappuoli (Novartis) discussed the applications of vaccines to viruses, bacteria and cancer. B. Chen (Harvard), B. Schief (Washington), and P. Kwong (Vaccine Research Center, NIH) highlighted diverse ways in which structural biology can address challenging stages of HIV-1 vaccine development, from epitope identification, to immunogen design and vaccine delivery.



The 2.9 Å structure of DdrB from *Deinococcus geothermalis*. Seiji Sugiman-Marangos, McMaster U.

Green Biochemistry: Focus here was on the production of biomass, carbon neutral biofuels, bioremediation, and biocatalysis. Three student presentations, B. Goblirsch (U. Minnesota), P. Chan (Toronto), and P. Cedervall, described structural and mechanistic studies of enzymes involved in bioremediation.

Crystallization Methods: B. Rupp stressed that modifying an obstinate protein is a more promising path to crystallization than additional screening. Z. Derewenda (U. Virginia) described how surface engineering can be used to obtain crystals of proteins otherwise recalcitrant to crystallization. B. Price (Columbia) analyzed the relationship between protein solubility and crystallization propensity and A. Dong (Toronto) discussed how excision of flexible loops and loose ends can facilitate crystallization. N. Seeman (New York) described the synthesis, construction, and X-ray diffraction analysis of 'designer' DNA crystals and their potential use for the development of drugs that interact specifically with defined sequences of DNA.

Chromatin Remodeling: New mechanisms for controlling post-translational modifications of histone proteins were highlighted and by combining crystallographic data and *in vivo* experimentation, R. Trievel (Michigan) identified a novel target for drug design to combat mycosial diseases.

Carbohydrate Recognition: Talks addressed design of multivalent carbohydrate mimetics as therapeutics for cystic fibrosis, A. Imberty (CNRS); specific inhibitors to control blood glucose levels in diabetes, L. Sim (Toronto), and α -mannosidase II target for inhibition of glycosylation in cancer metastasis, D. Rose (Waterloo/Toronto).



Mavis Agbandje-McKenna, Robert McKenna, John Domsic, Balendu Avvaru, Miorel Palii, Jeanne Quirit, Katherine Sippel and Balasubramanian Venkatakrishnan at the Opening Reception.

New Technology in Industry: Topics covered fragment based drug discovery, D. Davies (deCODE Biostructures), new developments in monochromator technology, R. Durst (Bruker-AXS), absolute configuration from Bijvoet differences of only C, H and N atoms, R. Scaringe (Bristol-Myers Squibb), and the effects of UV irradiation on protein crystal stability, P. Le Magueres (Rigaku).

Nanomaterials: Block copolymers (BCP) characterized by combining transmission electron microtomography and neutron reflectivity, H. Jinnai (Kyoto Inst. Tech.); anomalous swelling of polymer thin films induced by density fluctuations in supercritical carbon dioxide, P. Gin (SUNY Stony Brook - SAS SIG 2009 Etter Student Lecturer); constructing BCP-based supramolecules by associating small molecules to the side chain of one block, T. Xu (UC Berkeley); and polyelectrolyte layer-by-layer films, E. Kharlampieva (Georgia Tech.).

Cool Structures: E. Stevens (U. of New Orleans) described combining classical spectroscopic and charge density methods, and theoretical calculations to examine the exo-anomeric effect in an α,α -trehalose dihydrate.

Energy Related Materials: Two sessions covered hydrogen storage batteries and fuel cell related materials and *in-situ* characterization of thermoelectric and framework materials. M. Beekman (U. South Florida) presented his Etter Student Lecturer Award talk on intermetallic clathrates using X-ray powder diffraction.

Complementary Methods for Macromolecular Crystallography: Talks included computational techniques to interpret solution X-ray and neutron scattering data, D. Svergun (EMBL-Hamburg), and small angle X-ray scattering and cryoelectron microscopy, Dina Schneidman (UCSF). M. Hunter (Arizona State) described a study of Photosystem I in which a micro-jet device sent nanocrystals, containing only several thousand unit cells, into a soft X-ray beam while power diffraction patterns were recorded, demonstrating that fewer unit cells than have previously been used in micro-beam diffraction studies can give sufficiently strong diffraction to enable structural analysis.

Drug Design: P. Williams (Astex Therapeutics) discussed Fragment-Based Screening (FBS) to rapidly produce drug candidates; P. Colman (The Walter & Eliza Hall Inst.) talked about antivirals and the problem of drug resistance, and C. Abad-Zapatero (U. Illinois, Chicago) discussed new ways of plotting and analyzing FBS data. Etter Student Lecturer Ivan Campeotto (U. Leeds) discussed the use of directed

evolution to locate a mutation that increased substrate specificity and stereoselectivity of *N*-acetylneuraminic acid aldolase.

Superconducting Materials: Highlights included the description of the links between crystal structure and the maximum transition temperature in four families of Fe-based superconductors, D. Johrendt (Ludwig Maximilians U.), and charge doping as the critical parameter for superconductivity, S. Kimber (Helmholtz-Zentrum Berlin).

Refinement Software: Descriptions of the latest improvements to *REFMAC* and *autoBUSTER*, real space refinement and automated non-crystallographic symmetry in *MAIN*, and using *SHAKERR*, E. Pozharski (Maryland) were featured. A. Brunger (Stanford U.) described a deformable elastic network to restrain sampling to prior knowledge of an approximate or homologous structure.

Instrumentation: New sources, optics, robotics and detectors were described, including the Compact Light Source, a miniature synchrotron using inverse Compton scattering to produce X-rays; the new linac coherent light source at SLAC, the first hard X-ray free-electron laser beam whose extreme peak brilliance will permit use of nanometer-sized crystals; PILATUS 6M, the first large area pixel detector; beamlines at the Canadian Macromolecular Crystallography Facility that enable high-throughput and remote data collection; simultaneous, small and wide angle data collection on the X9 beamline at NSLS; a new robotics system to perform transfers, screening and data collection on frozen samples at the ESRF; microSAXS with microfluidics technology; and a time-resolved study at APS BioCARS that combined crystallographic and WAXS techniques. The Etter Student Lecturer J. Smith (Ottawa) described exploiting area detectors to reduce Compton scattering *via* energy selection and to measure beamline polarization.

Cooperative Phenomena in Magnetic Materials: D. Louca (Virginia) used neutron scattering to follow the development of magnetic superstructures in Cobaltites.

Large Small Molecules: G. Sheldrick (Göttingen) discussed dual space and charge flipping methods in the *SHELX* suite. Other talks concerned refinements of disordered (104 atoms) fullerene structures, M. Olmstead (UC Davis); successful phasing of a (2550 Da) molecule with one chlorine atom, P. Loll (Drexel); using neutron and X-ray diffraction data on deuterated crystals of rubredoxin to locate H atom positions, A. Gardberg (ORNL); incommensurately modulated structures with $Z' > 1$, C. Brock (Kentucky), and determining small protein structures by powder diffraction, P. Stephens (SUNY-Stony Brook).

Tips & Tricks of the Computing Trade: Speakers discussed a detailed description of twinned crystal indexing with *CELL_NOW*, G. Sheldrick; new visualization tools in the *ISAW* package for time-of-flight Laue single-crystal neutron diffraction, C. Hoffmann (ORNL); and development of the *GSAS* program suite, B. Toby (APS).

Accuracy and Standards in Powder Diffraction: Talks covered standards, requirements and certification procedures, J. Cline (NIST), and quantitative analysis of clay-containing minerals, O. Omotoso (NRC). Difficulties and possible strategies for overcoming them were reported, as was gauging the reliability of a Rietveld refinement using singular value decomposition to achieve the accuracy and precision of single-crystal techniques, P. Mercier (NRC).

Ferroic & Multiferroic Materials: V. Kiryukhin (Rutgers) described diode effects in single crystals of multiferroic BiFeO_3 in which the electric current is highly non-linear, temperature dependent, unidirectional and flowing in the same direction as the electric polarization; Etter Student Lecturer J. Wen (Brookhaven) discussed the unusual finding that an external magnetic field can affect the magnitude and correlation lengths associated with the charge order in LuFe_2O_4 , and C. Stock (Rutherford Appleton Labs, ISIS) described the structure of one of the most highly piezoelectric materials known. Ferroic materials include ferroelectrics, ferromagnets, and ferroelastics, whereas multiferroic materials are those in which two or more ferroic order parameters are present in a single phase; as such these materials possess enormous potential for industrial device applications.

Membranes and Associated Proteins: Topics ranged from cholesterol interactions with the lipid membrane to atomic resolution structures of membrane proteins. U. Perez-Salas (Argonne) discussed bicelle-based methods for membrane protein crystallization. M. Mueller (ETH Zürich) described the structure of the dodecameric membrane pore formed by cytolysin A and rearrangements that take place upon membrane insertion and pore formation.

Structural Enzymology: S. Liu (Pfizer) told how he took advantage of a less than stellar catalytic rate to trap intermediates and observe the reaction mechanism of a pharmaceutically important enzyme. Etter Student Lecturer A. Bah (Washington U.) combined classical enzymology and structural biology to engineer an allosteric switch into thrombin to help shut off the coagulation cascade. T. Maier (ETH Zurich) presented a movie illustrating how the substrate of the eukaryotic fatty acid synthases, a hetero-oligomeric structure, is shuttled from one reaction center to the next. IUCr President, Sine Larsen (U. Copenhagen), described substrate recognition and catalysis in polysaccharide lyases crucial to the clarification of apple juice. A. Kovalevsky (LANL) used time-of-flight neutron crystallography to determine exactly how xylose isomerase catalyzes the interconversion of glucose and fructose.

(Abstracted from ACA Reflexions, Fall 2009, pp. 10-46)

ACA Poster Prize Winners

- **Pauling** - C. Kimberlin (Scripps Inst.), Kristin Low (Queens U., Canada)
- **IUCr Prize** - C. McCrimmon (U. of Virginia)
- **Journal of Chemical Crystallography** - B. Vanchura II (Michigan State U.)
- **Protein Data Bank** - M. Korczynska (McGill U.)
- **Oxford Cryosystems** - M. Warren (U. Bath, UK)
- **AIP Undergrad. Research** - C. McCrimmon (U. of Virginia) and P. Carvalho Jr (Michigan State U.)

MEETING REPORT

ECM25

Istanbul, Turkey, August 2009. www.ecanews.org

André Authier delivers his Historical Overview at ECM25.

The 25th European Crystallography Meeting had a special significance for Organizers and Participants of the meeting as well as the European Crystallographic Association itself. Thus, along with the usual microsymbposia, plenary lectures, an Opening Ceremony and meetings of the ECA Council, the ECA Executive and the SIGs, a special ceremony to mark the 25th Anniversary. André Authier, first Chairman of the European Crystallographic Committee, presented a Historical Overview of the formation of the ECA and its early history. This lecture has been published in *Acta Cryst. A* **66**, 1-4: *The birth of the European Crystallographic Committee (ECC) and of the European Crystallographic Meetings (ECMs)*.

The distribution of oral and poster presentations in the major categories of crystallographic research was as follows: (the first percentage being the oral presentations and the second being the posters).

Biological and Macromolecular Crystallography (29%, 21%); Materials and Minerals (23%, 21%); Physical including fundamental crystallography (8%, 5%); Chemical Crystallography (25%, 40%); Experimental and Computational techniques (15%, 13%). These five ECM Focus Areas map onto the thirteen ECA SIGs (see www.ecanews.org/sig_approved.php). Overall there were a total of 235 and 482 oral and poster presentations and the participants came from 51 countries. There was also a *Crystallographic Software Fayre* organized by Martin Lutz, as well as a Commercial Exhibition comprising 27 exhibitors. There were a total of 71 student bursaries awarded, which were supported financially by the following sponsors: the IUCr, ECA, the Turkish Crystallographic Association (TCA), the Turkish Scientific and Technical Research Council (TUBITAK) and the Organization for the Prohibition of Chemical Weapons (OPCW), comprising a total of \$12000 and 12000 Euros.

Added to this program the usual awards for the Perutz Prize and the Bertaut Prize were both made. The details of these have been published in a previous *IUCr Newsletter* and are also available on the ECA website: www.ecanews.org/ecaprize.php. There are now also a wide variety of ECM Poster Prizes and the recipients and sponsors of these Prizes are summarised at www.ecanews.org/posterprize.php. These latter Prizes were presented at the ECM25 Closing Ceremony.

A Satellite Conference on Mathematical and Theoretical Crystallography, *Symmetry and Crystallography in Turkish Art and Culture*, organized by Massimo Nespolo, was held immediately before ECM25, also at the Istanbul Military Museum and Congress Centre.



Swirling Dervishes at the Church of St Irene.



Gala Dinner in the grounds of the Dolmabahce Palace.

The Social Program was able to draw on the rich and diverse culture and buildings of Istanbul. A concert was held at the Church of St Irene and included both orchestra and Whirling Dervishes performances (the latter pictured). The Gala Dinner was held at the Dolmabahce Palace followed by dancing by the diners. The Excursion Day, *i.e.* the day after the Scientific Conference had concluded, was a Bosphorus Cruise. In addition Turkish Military Orchestra and Turkish Dance performances were given at the Opening Ceremony and the 25th Anniversary evening respectively.

Overall, the 805 Delegates, the 75 Accompanying Persons and the 70 Exhibitor Representatives enjoyed a truly memorable scientific and cultural program.



Leaders of the British (Susanne Huth (now Coles) centre) and Spanish Young Crystallographers (Laura Rocés and Laura Torre-Fernandez, centre left and right respectively) with ECA President John Helliwell and ECA Incoming President Santiago Garcia-Granda left and right at ECM25.

In terms of new initiatives for the ECA it was a pleasure to formally host the Young Crystallographers at the Istanbul Technical University Guest House poolside (the Leaders of the British and Spanish Young Crystallographers are pictured with the ECA outgoing and incoming Presidents).

Engin Kendi, John R. Helliwell, Suheyra Ozbey and Semra Ide on behalf of the ECM25 Local Organizing Committee and the Programme Committee as well as the ECA.

MEETING REPORT

High-Pressure Crystallography: From Novel Experimental Approaches to Cutting-edge Technologies

Erice, Italy, June, 2009, www.crystallalice.org/



The 2009 Erice school on high-pressure research was co-directed by Elena Boldyreva (Novosibirsk, Russia) and Przemek Dera (Chicago, USA) and supported by the IUCr Commissions on High-Pressure, Teaching, Inorganic and Mineral Structures. The school was attended by 122 participants from USA, UK, Germany, France, Italy, Russia, Poland, Spain, Sweden, China, India, Netherlands, South African Republic, Israel, Switzerland, Belarus, Nigeria, Ukraine, Czech Republic, Colombia, Brazil, and Portugal. With respect to gender distribution, 8 out of 46 speakers, and 44 out of 122 participants were female and 20% of invited speakers were younger than 35 years of age.

The topics covered included: physics (properties and structure), chemistry (chemical reactions, transport), materials science (new materials), and engineering (mechanical properties), implications for geology (minerals in their natural, deep earth environments), planetary sciences, biology and medicine. In addition, direct or indirect (e.g. economic) applications of high-pressure science in several fields of modern technology have been considered. Such a variety of topics produced a 'densely packed' program which 'kept the participants under pressure' for 10 days.



Formal presentations included a general introduction to high pressure science (P. Dera, USA), principles of operation of the diamond anvil cells (M. Paz-Pasternak, Israel), large volume press techniques (Yanbin Wang, USA), synchrotron X-ray diffraction at high pressure, including high- and low-temperature research (M. Mezoua, France and P. Dera, USA), Mossbauer and high-resolution inelastic scattering (J. Jackson, USA), X-ray absorption spectroscopy (J.-P. Itie, France), different approaches to measuring transport properties under pressure (L. Dubrovinsky, Germany), plastic properties, texture analysis, elasticity, plasticity and rheology of minerals and materials (S. Merkel, France and Y. Wang, USA), and high-intensity and high-resolution neutron diffraction and scattering at high pressure (A. Balagurov, Russia and J. Loveday, UK). Other lectures emphasized applications of these techniques and approaches. In the workshops the students were taught how to adjust a DAC, load a sample into the DAC and crystallize a liquid in it (C. Pulham, UK, assisted by K. Dziubek, Poland, and G. Hearne, South Africa), how to treat high-pressure X-ray powder diffraction data (Y. Filinchuk, France), how to obtain reliable and correct data on the equation of state (T. Boffa-Balaran, Germany), and calculations of crystal structures and properties at high pressures using different algorithms (A. Oganov, USA and P. Macchi, Switzerland). Handouts with detailed explanations of the procedures were provided, and the participants had an

opportunity to use the software on the computers at the Ettore Majorana Center, as well as their own laptops.

A round-table discussion on the improvement of data collecting and processing was organized by N. Casati (Italy) assisted by F. Fabbiani (Germany), K. Dziubek (Poland), and P. Dera (USA). An important outcome of the 'round table' was the birth of three new online Digital Resources for High Pressure Crystallography (DigResH-PX). The DigResHPX package includes: a High Pressure Crystallography blog: <http://hpdac.net/>, mailing list: hpdac@hpc.amu.edu.pl, and a wiki: cars9.uchicago.edu/surfacewiki/HPCrystallography. These online tools and services provide a communication platform for exchange of technical information, advice, references, discussions etc. for high-pressure crystallography. The poster sessions were preceded by short oral presentations of all 52 posters.



This year the tradition of a virtual course was continued by J. Irwin (USA), K. Dziubek and A. Budzianowski (Poland). The lectures were broadcast to several countries. Despite a 5 hour time difference 30 people followed the lectures in Novosibirsk, thanks to the cooperation of JointLab Director A. Arzhannikov and REC-008 Director V. Boldyrev of the Novosibirsk State U. Technical. The support of N. Zanin (Centre of the New Information Technologies NSU), and the organizational efforts of Anna Nartova (REC-008) are gratefully acknowledged. Most of the lectures can be downloaded from the HPCrystallography wiki (see DigResHPX above). A book will be published as part of the *NATO Science for Peace and Security Series: B – Physics and Biophysics* by Springer.

The team of 'orange scarfs' (A. Guerri, I. Doverbratt, A. Olejniczak, A. Idczak, E. Papinutto, M. Lusi, and F. Nicoli) led by Lodovico Riva di Sanseverino (Bologna, Italy), Paola Spadon (Padova, Italy) and J. Irwin (UCSF, USA) did a great job of organizing the meeting. As one of the participants commented: 'All we participants had to do was to be on time. The organizers did the rest of the job'.

Elena Boldyreva, Paola Spadon and Przemyslaw Dera

MEETING REPORT

XXI Conference on Applied Crystallography

Zakopane, Poland, September, 2009, www.cac.us.edu.pl



As with all the previous conferences, this one was organized by the Inst. of Material Science of the U. of Silesia in Katowice. The Honorary Chairman of the Conference was Henryk Morawiec (Poland) and the Chairman was Danuta Stróz (Poland).

The conference was followed by the PDF4+ Users Workshop (September 24-25) directed by Matteo Leoni, Regional Co-chairman for Europe (Italy), Paolo Scardi, ICDD Director-at-Large (Italy), and Cyrus Crowder, ICDD Principal Scientist (USA). The other satellite events were the Summer School on Polycrystalline Structure Determination under the direction of Carmelo Giacovazzo (Italy) and the Summer School on Diffraction-based Structure Analysis in TEM under the direction of János Lábár (Hungary) (September 25-27).

The Committee of Crystallography and the Committee of Material Science of the Polish Academy of Sciences were the co-organizers of the events. The IUCr awarded scholarships to enable young scientists to attend the conference and the schools. The conference was also sponsored by the Polish Academy of Sciences.

A total of 120 delegates from 12 countries gathered and engaged in lively discussions throughout the plenary, oral and posters sessions. There were 12 plenary and 27 oral lectures and 67 posters were displayed. The plenary lectures were given by prominent scientists in the field of crystallography and structural studies, Andrew Fitch (France), Carmelo Giacovazzo (Italy), Bogdan Kotur (Ukraine), János Lábár (Hungary), Jean-Paul Mornirolli (France), Reinhard Neder (Germany), Vaclav Petricek (Czech Republic), Paolo Scardi (Italy), Lubomir Smrcok (Slovakia), Marek Wolcyrz (Poland) and others.

The topics included development of methods and techniques in the crystal structure determination methods, crystallography of phase transformations, texture analysis, material structures – metals and alloys, ceramics, polymers, thin films, quasi-crystals, amorphous materials, nanomaterials, and molecular crystals. The conference proceedings will be published in the *Solid State Phenomena*, Trans Tech Publications in Switzerland.

The organizers also took care of the social aspects, including an excursion to Chocholów, the village in the Tatra Mountains, which is comprised almost exclusively of the original Polish 'Góral' highlanders' wooden houses. Conference photos can be viewed on the website.

The next, XXII CAC will be organized in September 2012.

Malgorzata Karolus

MEETING REPORT

On-line Brillouin Spectroscopy

Argonne, IL USA, September 2009 cars.uchicago.edu/gsecars/dac_brillouin_workshop/brillouin_workshop.htm

GeoSoilEnviroCARS hosted the workshop 'On-line Brillouin Spectroscopy: Basic Principles and Application for High Pressure Research' at the Advanced Photon Source (APS). The workshop was attended by 48 researchers in high pressure science, including graduate students, postdoctoral fellows, and participants from outside the US. Talks focused on fundamental aspects of Brillouin scattering and the challenge of combining Brillouin spectroscopy with synchrotron X-ray diffraction techniques, including single-crystal, micro-/nanocrystalline, and amorphous materials. Descriptions of the existing high pressure Brillouin spectroscopy facilities in USA, Germany, Switzerland and Japan, and descriptions of alternative techniques for measuring sound velocities at high pressure and temperature, were presented.



Participants at the On-line Brillouin Spectroscopy Workshop. Row 1: Jane Andrew, Anastasia Kantor, Stas Sinogeikin, Yuming Xiao, Gopal Pradhan, Nadege Hilairret, Yun-Yuan Chang, Sylvia-Monique Thomas (front), Yue Meng (back), Vitali Prakapenka. Row 2: Carmen Sanchez-Valle, Jay Bass, Tony Yu, Chang-Sheng Zha, Greg Finkelstein, Lili Gao, Esen Alp, Marcos Grimsditch, Zeyu Li. Row 3: Jue Wang, Simon Clark, Przemek Dera, Hyunchae Cynn. Row 4: Wenge Yang, Yanbin Wang, Justin Hustoft, Alexander Goncharov, Nagayoshi Sata, Jiachao Liu, Bin Chen, Xinyang Chen. Row 5: Alexander Kurnosov, Inno Kantor. Row 6: Jonathan Crowhurst, Steve Sutton, Pavel Zinin, Baosheng Li, Dattatraya Dandekar, Chris Holl. Not pictured: Malcolm Guthrie, Valentin Iota, Jung-Fu Lin, Zhu Mao, Olga Shebanova, Guoyin Shen, Wolfgang Sturhahn, Brian Toby, Jiyong Zhao.

The workshop included a tour of high pressure beamlines at the APS and a demonstration of capabilities at GSECARS. Over half of the attendees participated in a hands-on session on the last day. Data analysis software was provided to all participants. The workshop was organized by Vitali Prakapenka (GSECARS, U. of Chicago), Jay Bass (U. of Illinois at Urbana-Champaign), and Stanislav Sinogeikin (HP-CAT, Carnegie Inst. of Washington), with assistance from Nancy Lazarz and Jane Andrew (U. of Chicago). The organizers acknowledge the support of the Consortium for Materials Properties Research in Earth Sciences (COMPRES), Princeton Instruments, the Center for Advanced Radiation Sources of the U. of Chicago and the Argonne National Laboratory.

Vitali Prakapenka and Jane Andrew

OBITUARY

Louis T. J. Delbaere (1943-2009)

Louis T. J. Delbaere died suddenly on October 5 in Mississauga. He was born in St. Boniface, Manitoba. He received his BSc. and his PhD. in Chemistry from U. of Manitoba. Louis began working as a mineralogist crystallographer. During a post-doctoral fellowship in Oxford he characterized the covalent linkage between carbohydrates and proteins.

During a postdoctoral fellowship at the U. of Alberta, Louis made a major contribution to understanding the structural features of the human Lewis blood-group determinants. Later, Louis was a key figure in our successful determination of the first protein structure to be done in Canada, that of *Streptomyces griseus* protease B (SGPB). (Louis worked with Gary Brayer on the structure of α -lytic protease and with I-Nan Hsu on penicillopepsin). Louis had a passion for attending horse races that almost matched his passion for science. There were many gatherings at the Delbaere home celebrating varied occasions. Louis and Carol had a very closely-knit family and their friendship and happiness was shared with all.

Taken from ACA Reflexions, Winter 2009

Louis in the Biochemistry Dept., U. of Saskatchewan

In 1979, Louis moved to the Biochemistry Dept. of the University of Saskatchewan in Saskatoon to start the first protein crystallography lab at the University. In 1988, Louis and I obtained a synchrotron data set at the EMBL outstation at DESY in Hamburg that gave a publishable structure. Louis grew the first Canadian crystal in space. In the mid 1990's, Saskatoon was selected as the site for a Canadian synchrotron. Louis organized mini-symposia on synchrotron applications around the country with members of the granting agencies and lobbied scientists in other areas that might use synchrotron radiation. Amazingly, it all came together and the Canadian Light Source (CLS) is now in Saskatoon. Louis was the project leader for the first protein crystallography beam-line at the CLS. He had been the Chair of the Canadian National Committee for the IUCr since 2005. He was President of the ACA in 2005. At the Osaka IUCr meeting in 2008, he successfully led the committee promoting Montreal as the site for the IUCr meeting in 2014 and he had recently been elected for a six-year term to the Executive Committee of the IUCr.

Wilson Quail

Louis as Supervisor and Mentor

Louis supervised or co-supervised seven PhD students, eight Masters, five postdoctoral fellows and research associates, a number of technicians and countless undergraduate honors projects and summer students. To his students, he was a mentor and a friend. Louis' style was one of quiet enthusiasm and encouragement. He was always available to discuss problems, directions and the latest crazy ideas that we'd come up with. He taught us to follow the data, be open to various viewpoints and methods, be patient and to 'trust the electron density ... it doesn't lie'. He instilled a passion to make sure that the correctness of the analysis and the crystallography, rather than the flash of the story, was what was critically important. He taught us not to overinterpret the data, but to make sure it was correct, and move forward confidently in addressing our hypotheses. He encouraged everyone to be a member of the ACA, and to present posters at least once a year at a conference. These conferences were primarily the

annual ACA meeting, but also included the IUCr congress, various Canadian meetings and the Erice meetings. Louis would make a point of introducing all his students to his colleagues during poster sessions and other formal and informal situations; we've all ended up with international networks of professional contacts and colleagues.

Gerald F. Audette

Louis and the IUCr

The participants in Osaka remember well Louis' happiness when Montreal was selected as the site of the 2014 IUCr meeting. It was clear that he looked forward to welcoming crystallographers from all over the world to Montreal. Another important election that took place at the Osaka Congress was the one that made Louis a member of the IUCr EC. After a few months he took on the important task of chairing the IUCr Sub-committee on the Union Calendar, which handles applications for support for international crystallographic meetings. Louis chaired the Committee efficiently and with great understanding for the importance of distributing the 150,000 US dollars in a way that promotes crystallography worldwide. Global awareness was more than a 'buzz word' to Louis, he was known and respected by crystallographers all over the world and was an excellent representative of the 'Americas'.

Sine Larsen

OBITUARY

Dominique Grebille (1957-2009)



Dominique Grebille passed away on January 27, 2009, at the age of 51, in Caen. He received an engineers diploma from the Ecole Centrale (Paris) in 1980, joined the Chimie-Physique du Solide Laboratory and defended his PhD entitled 'Etude de produits boehmitiques peu cristallisés obtenus à partir de gels d'oxychlorure d'aluminium' in 1982. At that time, military service was still an obligation in France, unless you performed alternate services. For two years he taught Braille at the Group of Blind and Amblyopic Intellectuals, a skill which he used to help others throughout his working life. Dominique became an assistant professor at the Ecole Centrale, teaching physics and crystallography, and habilitated in 1992. He joined the CRISMAT Laboratory at ENSICEAN as full professor, and animated the crystallography team.

His main research interest was in modulated, incommensurate, composite and aperiodic structures of superconductors, magnetoresistive or thermoelectric compounds. He was a pioneer in the analyses of new commensurate and incommensurate structures of high temperature superconducting oxides. For this analysis he developed new crystallographic tools. His studies of modulated, and composite crystals using the superspace formalism are among the most highly regarded. Recently, he concentrated on high resolution characterization of multilayers and superlattices exhibiting multiferroic properties, and materials irradiated by heavy ions. He has more than 75 publications in international journals.

Dominique was a kind and generous teacher who supervised eight PhD students now working in various laboratories. He served the crystallographic community as vice president of the French Crystallographic Assn, by organizing a crystallographic congress in Caen, and conducting an employment survey involving crystallographers in many fields of science and industry. Dominique was a brilliant scientist, a modest humanitarian, and a gentle human being who was supportive of the blind and critical of bureaucracy. His premature death ends a brilliant career, but his spirit will remain in our memory forever.

Olivier Pérez, Daniel Chateigner, and Jean-François Berar

AWARDS AND PRIZES

ACA 2010 Award Winners



Anthony L. Spek

The American Crystallographic Association has announced its 2010 award winners. Anthony L. Spek (Utrecht U. Bijvoet Center for Biomolecular Research) has been selected to receive the 2010 Kenneth Trueblood award for his outstanding contributions to chemical crystallography and crystallographic computing.



David Watkin

David Watkin (Oxford U.) is the recipient of the 2010 Isidor Fankuchen Award for his stewardship of the crystallographic software package *CRYSTALS* for X-ray structure refinement and analysis. The worldwide success of *CRYSTALS*, used by students, academics and industrial users alike, can be attributed to its ease of use and to Watkin's unceasing support of the software and its users.



Raymond C. Trievel

Raymond C. Trievel (U. of Michigan) received the 2010 Margaret C. Etter Early Career Award for his achievements in elucidating the substrate specificity and catalytic mechanism of histone methyltransferases in the short time that he has been an independent researcher. The awards will be presented at the ACA meeting in Chicago, IL, July 24-29, 2010.

AWARDS AND PRIZES

Iijima Receives Japan's Top Cultural Award



Sumio Iijima (Senior Research Fellow at NEC Corporation, Professor of Meijo U., Research Director of the International Cooperative Research Project at the Japan Science and Technology Corporation (JST), and Director of the Research Center for Advanced Carbon Materials at the National Institute of Advanced Industrial Science and Technology (AIST)) has been selected to receive The Order of Culture (bunka kunshō, Japan's top cultural award). Japanese Government recognizes Dr. Iijima's contributions to the development of high resolution electron microscopy and discovery of carbon nanotubes.

In 1991, using advanced electron microscopy techniques, he discovered the needle crystal which was synthesized on a carbon electrode subjected to arc discharge. He then clarified that the crystals are made of carbon with a cylindrical nanostructure, and called them nanotubes. Dr. Iijima opened a global research field of carbon nanotechnology from basic materials science to practical applications.

The Order of Culture is given to the people who contribute to art, literature or culture in Japan. In 2009, only 5 people were selected. The Order was presented at the ceremony held in the Imperial Palace on November 3, 2009.

Tsuyoshi Inoue

LETTER TO THE EDITOR

Letter to the Editor

CrysAC and C.P. Snow

In his article introducing the new Commission on Crystallography in Art and Cultural Heritage (CrysAC), linking crystallography and artistic expression (IUCr N/L 16, No3, pp5-6, 2008), Cele Abad-Zapatero refers to the English novelist C.P. Snow. It is just half a century since Snow introduced the phrase 'The Two Cultures', referring to the apparent divide between literary intellectuals and scientists.

Snow conducted research at Cambridge, in the 1930s and became a great friend of J.D. Bernal. Following war time work as a scientist, Snow became a senior official in the Civil Service. His experience in the corridors of power formed the background to his novels, including *The Search* (1934) in which the narrator begins his research in X-ray crystal-structure analysis. The model for the brilliant scientist 'Constantine' is clearly J.D. Bernal. Constantine was an amorous eccentric with big hair and an immense classical knowledge who envisaged an international team of biologists, chemists and physicists tackling proteins at a dedicated institute. Snow is quoted, together with an extract from Bernal's 1937 paper on architecture and science in the entertaining and scholarly book *In our own image: personal symmetry in discovery* by Istvan and Magdolina Hargittai (Kluwer, 1999). In this book, black and white images by graphic artist Istvan Orosz accompany personal stories of outstanding scientists (predominantly crystallographers) who made the main conceptual advances in our perception of the aesthetic intellectual area of symmetry.

Derry W. Jones